

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
 Data File : BG055456.D  
 Acq On : 4 Nov 2022 16:20  
 Operator : CG/JU  
 Sample : N5306-10  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055456.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 5.274       | 333           | 338         | 350          | rBV      | 21986          | 35517         | 1.81%           | 0.438%        |
| 2         | 5.756       | 414           | 420         | 437          | rVB      | 193741         | 343191        | 17.48%          | 4.236%        |
| 3         | 7.383       | 690           | 697         | 710          | rBV      | 154424         | 282968        | 14.41%          | 3.493%        |
| 4         | 8.229       | 835           | 841         | 855          | rBV      | 83614          | 150464        | 7.66%           | 1.857%        |
| 5         | 9.410       | 1033          | 1042        | 1063         | rVB      | 244227         | 448915        | 22.87%          | 5.541%        |
| 6         | 10.808      | 1274          | 1280        | 1294         | rBV      | 43168          | 88759         | 4.52%           | 1.096%        |
| 7         | 11.061      | 1316          | 1323        | 1332         | rBV      | 124460         | 216380        | 11.02%          | 2.671%        |
| 8         | 13.476      | 1727          | 1734        | 1743         | rBV      | 791461         | 1191450       | 60.69%          | 14.707%       |
| 9         | 14.851      | 1958          | 1968        | 1977         | rBV      | 209018         | 336823        | 17.16%          | 4.158%        |
| 10        | 16.331      | 2214          | 2220        | 2234         | rBV      | 659818         | 1013639       | 51.63%          | 12.512%       |
| 11        | 17.583      | 2427          | 2433        | 2445         | rVB      | 313671         | 455406        | 23.20%          | 5.621%        |
| 12        | 18.206      | 2535          | 2539        | 2546         | rBV3     | 24956          | 36077         | 1.84%           | 0.445%        |
| 13        | 18.435      | 2573          | 2578        | 2587         | rBV2     | 33332          | 57290         | 2.92%           | 0.707%        |
| 14        | 19.363      | 2732          | 2736        | 2743         | rVB2     | 30525          | 38668         | 1.97%           | 0.477%        |
| 15        | 20.156      | 2865          | 2871        | 2877         | rBV      | 1525710        | 1963173       | 100.00%         | 24.233%       |
| 16        | 21.461      | 3086          | 3093        | 3107         | rBV6     | 28672          | 110134        | 5.61%           | 1.359%        |
| 17        | 21.854      | 3154          | 3160        | 3167         | rBV      | 330695         | 538645        | 27.44%          | 6.649%        |
| 18        | 23.546      | 3441          | 3448        | 3456         | rBV      | 109802         | 217226        | 11.07%          | 2.681%        |
| 19        | 25.227      | 3724          | 3734        | 3749         | rVB      | 192248         | 576626        | 29.37%          | 7.118%        |

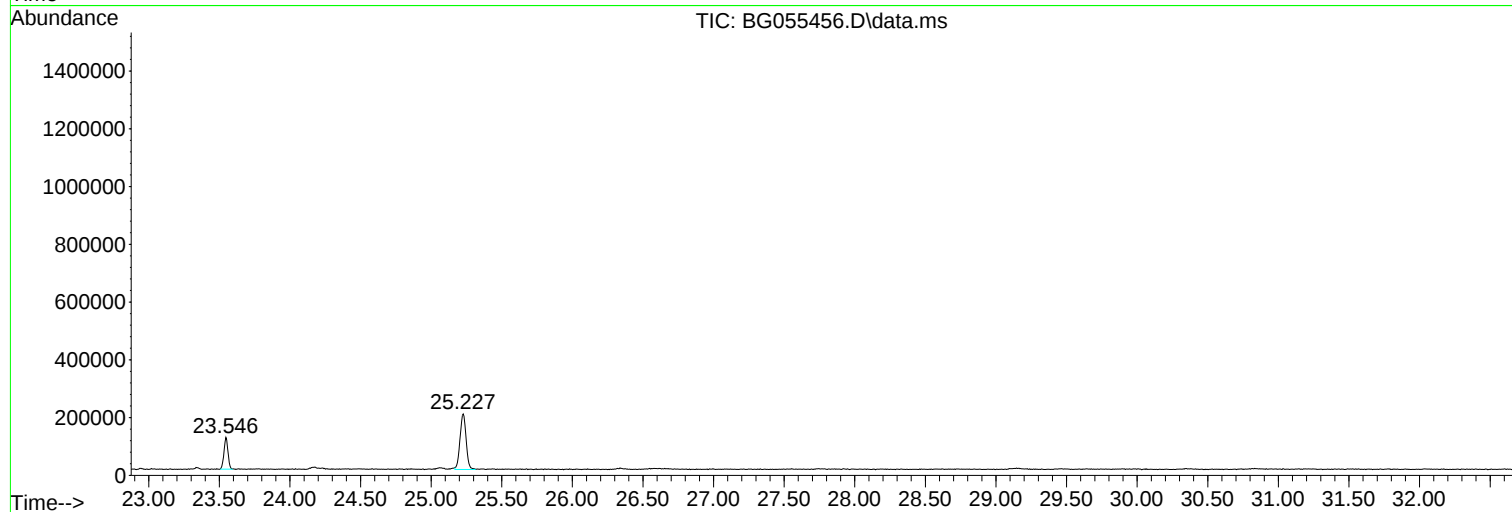
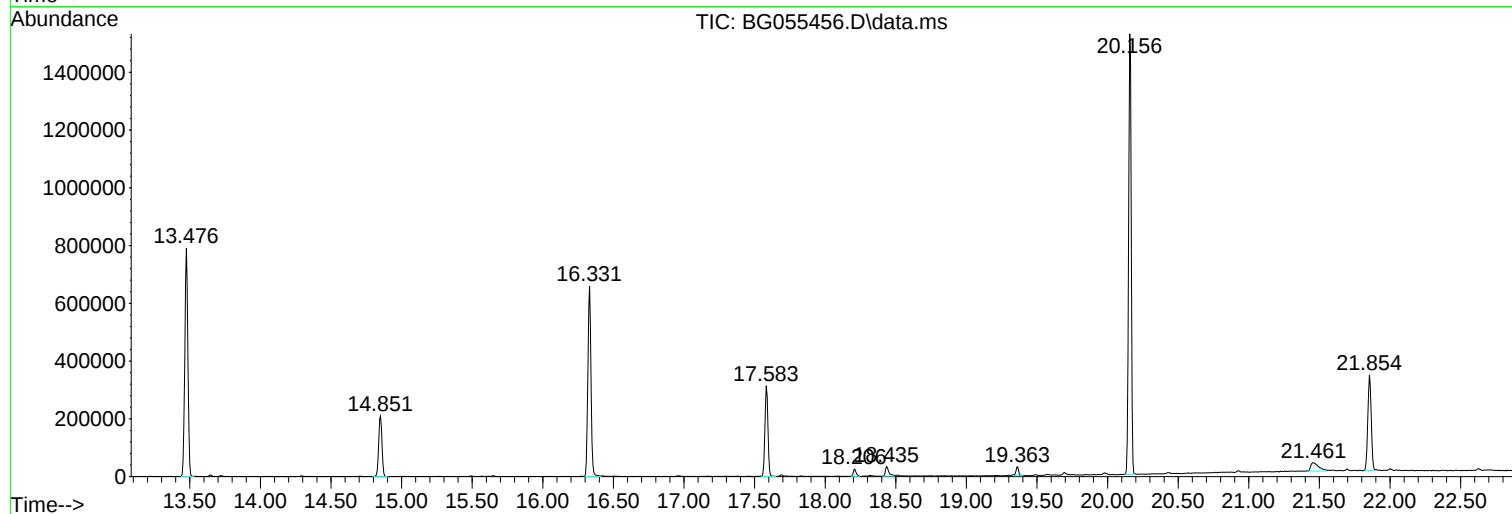
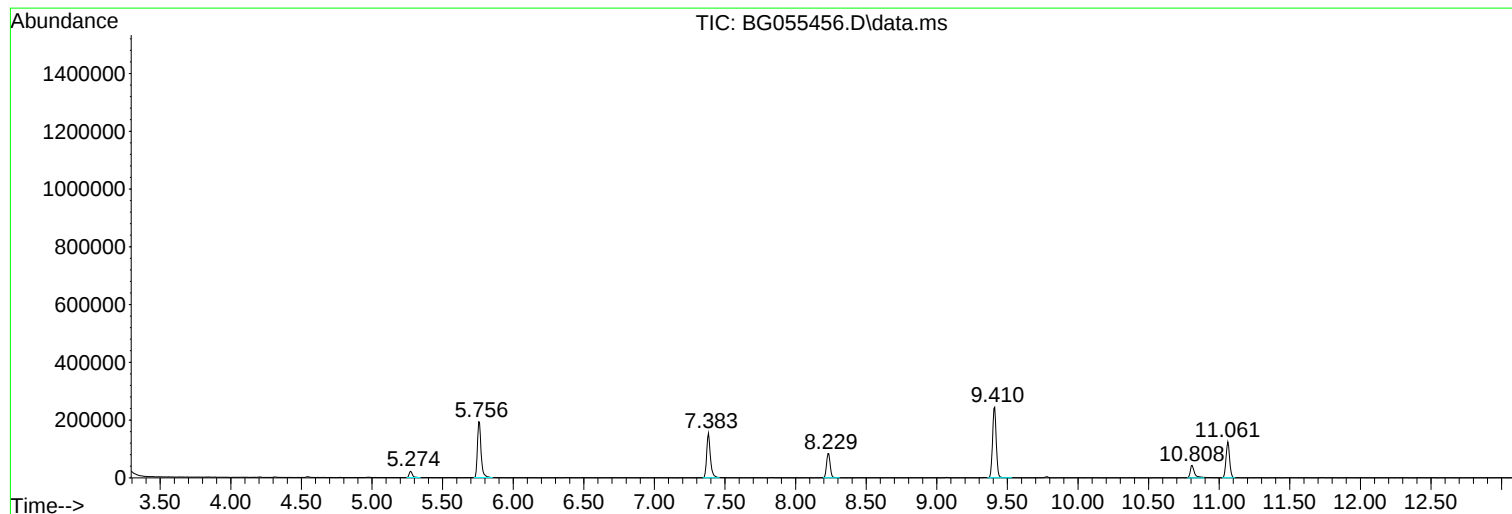
Sum of corrected areas: 8101351

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

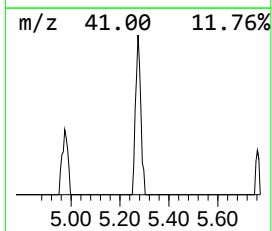
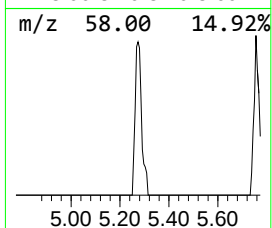
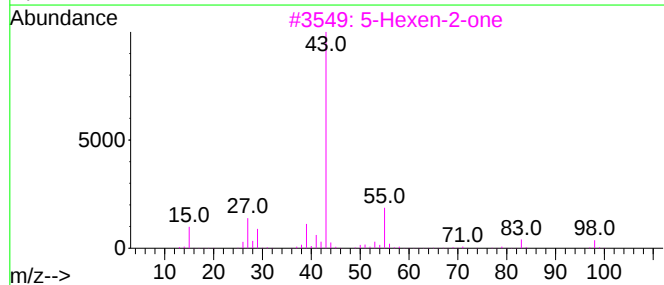
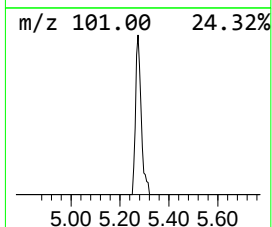
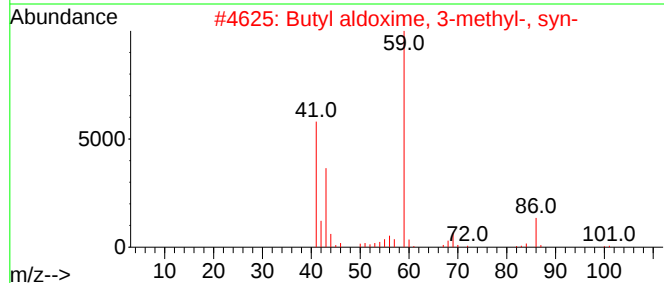
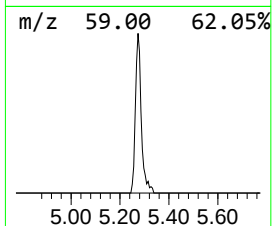
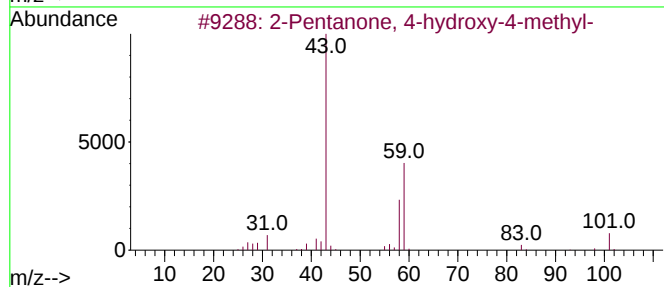
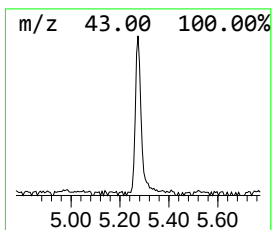
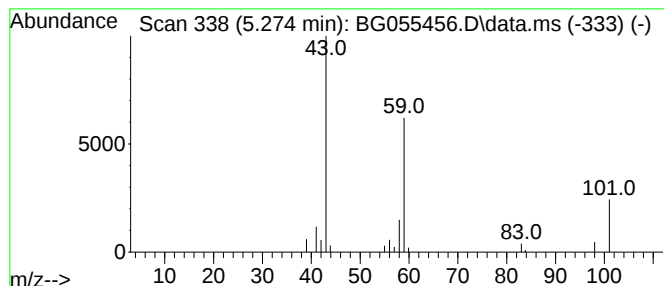
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.274 | 4.72 ng | 35517 | 1,4-Dichlorobenzene-d4 | 8.235 |

| Hit# | of 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|------|----------------------------------|-----|---------|-------------|------|
| 1    |      | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 72   |
| 2    |      | Butyl aldoxime, 3-methyl-, syn-  | 101 | C5H11NO | 005780-40-5 | 25   |
| 3    |      | 5-Hexen-2-one                    | 98  | C6H10O  | 000109-49-9 | 9    |
| 4    |      | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6 | 9    |
| 5    |      | 1-Propen-2-ol, acetate           | 100 | C5H8O2  | 000108-22-5 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

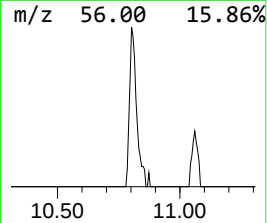
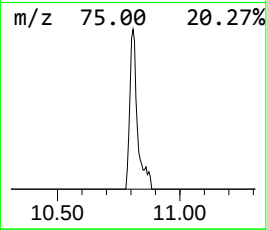
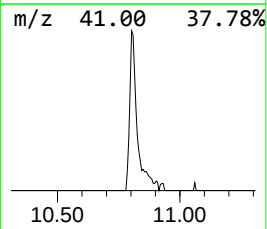
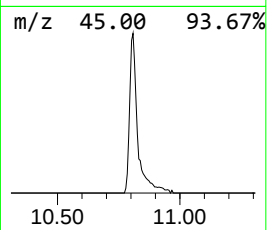
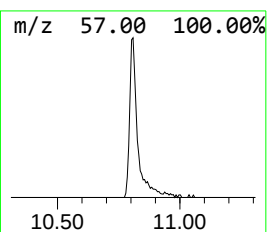
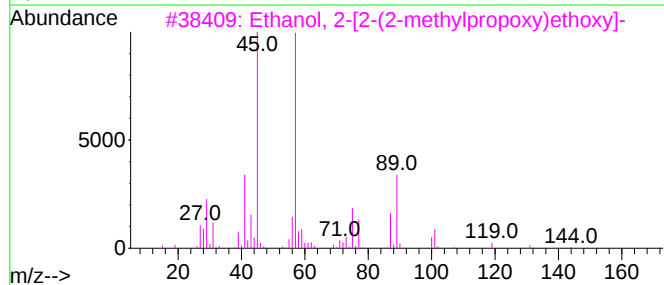
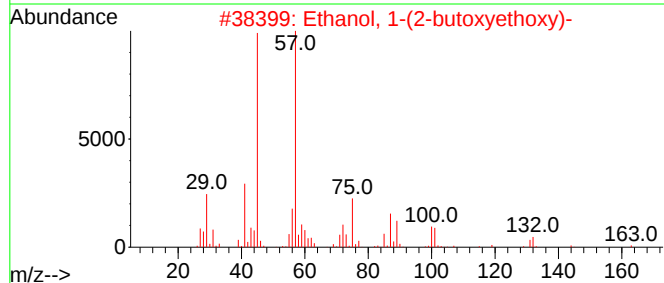
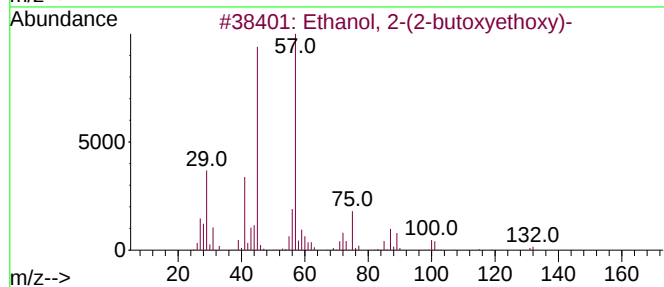
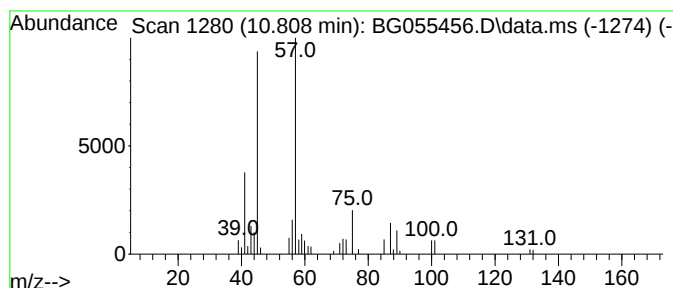
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|-------|------------------|-------------|------|
| 10.808    | 8.20 ng                             | 88759 | Naphthalene-d8   | 11.061      |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#        | Qual |
| 1         | Ethanol, 2-(2-butoxyethoxy)-        | 162   | C8H18O3          | 000112-34-5 | 90   |
| 2         | Ethanol, 1-(2-butoxyethoxy)-        | 162   | C8H18O3          | 054446-78-5 | 90   |
| 3         | Ethanol, 2-[2-(2-methylpropoxy)e... | 162   | C8H18O3          | 018912-80-6 | 72   |
| 4         | Ethylene glycol monoisobutyl ether  | 118   | C6H14O2          | 004439-24-1 | 64   |
| 5         | Tetraethylene glycol                | 194   | C8H18O5          | 000112-60-7 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

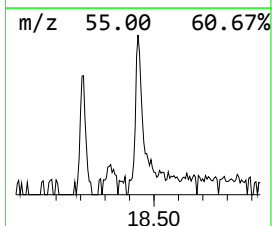
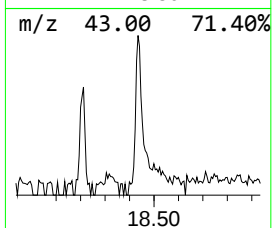
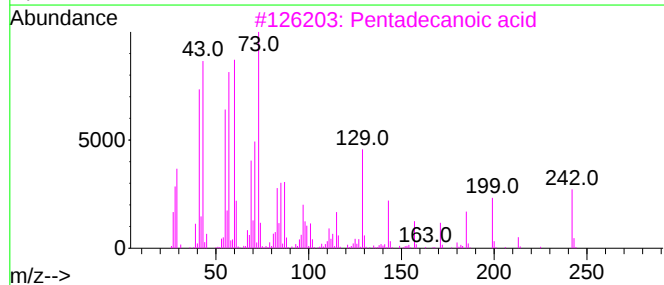
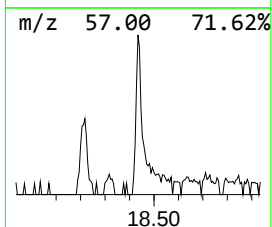
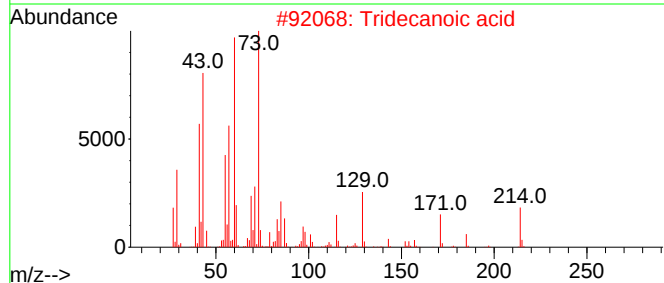
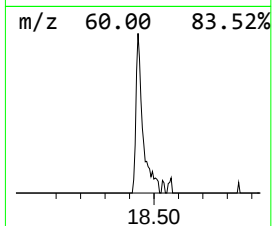
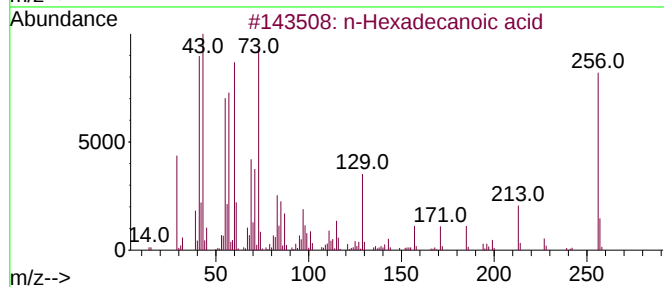
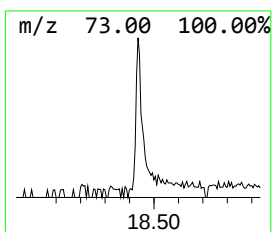
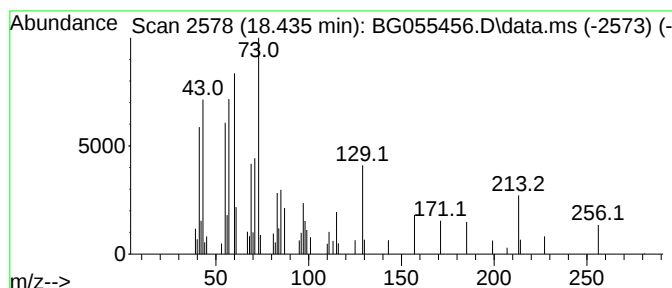
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 18.435 | 2.52 ng | 57290 | Phenanthrene-d10 | 17.583 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3  | 98   |
| 2    |    |   | Tridecanoic acid                    | 214 | C13H26O2 | 000638-53-9  | 94   |
| 3    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2  | 83   |
| 4    |    |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5  | 64   |
| 5    |    |   | .beta.-D-Mannofuranoside, 1-O-(1... | 332 | C17H32O6 | 1000155-29-9 | 14   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

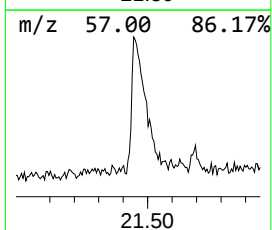
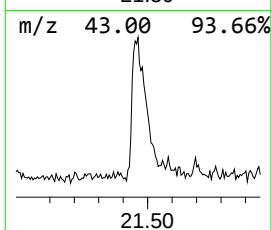
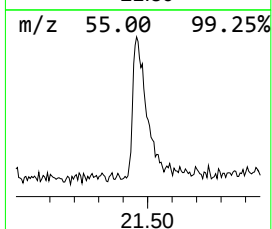
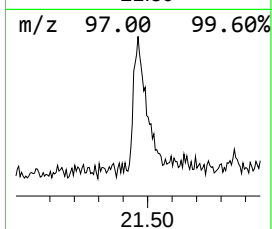
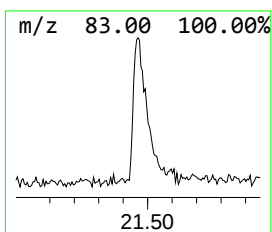
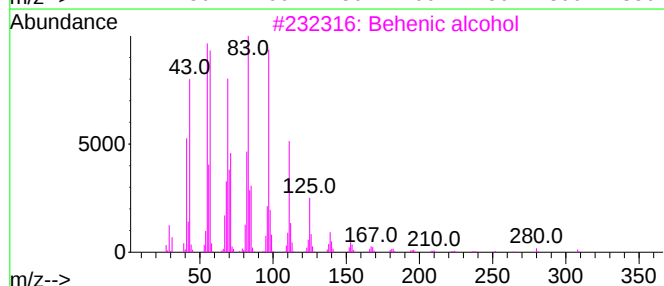
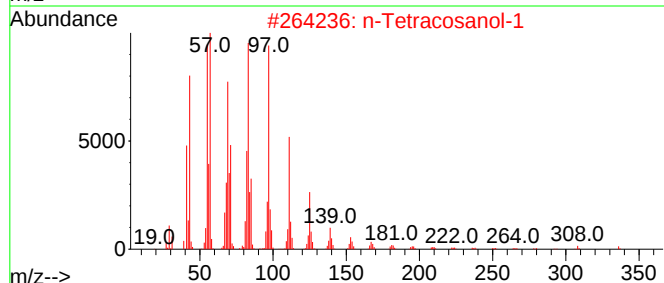
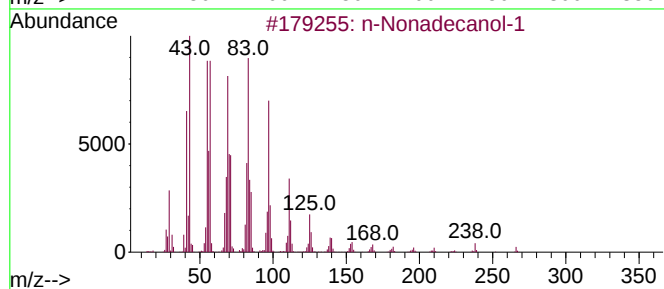
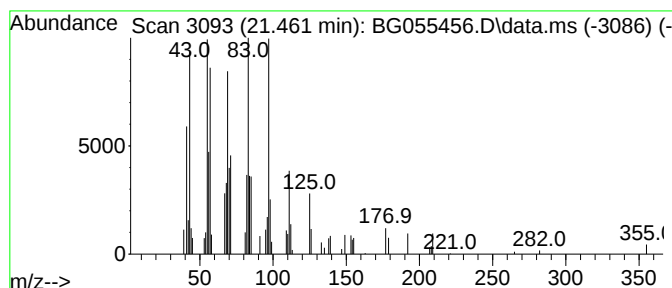
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 4 n-Nonadecanol-1 Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.461 | 4.09 ng | 110134 | Chrysene-d12     | 21.854 |

| Hit# | of 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|------|------------------|-----|---------|-------------|------|
| 1    |      | n-Nonadecanol-1  | 284 | C19H40O | 001454-84-8 | 93   |
| 2    |      | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 91   |
| 3    |      | Behenic alcohol  | 326 | C22H46O | 000661-19-8 | 91   |
| 4    |      | 11-Tricosene     | 322 | C23H46  | 052078-56-5 | 91   |
| 5    |      | 1-Heneicosanol   | 312 | C21H44O | 015594-90-8 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

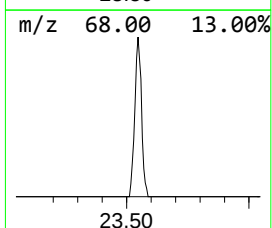
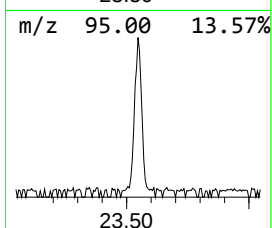
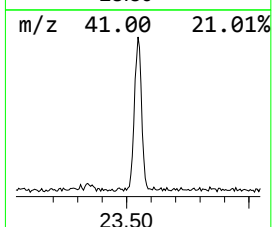
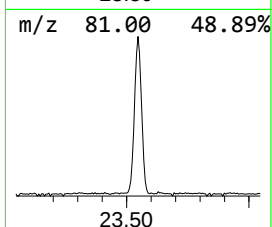
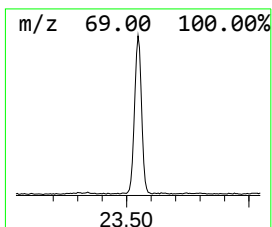
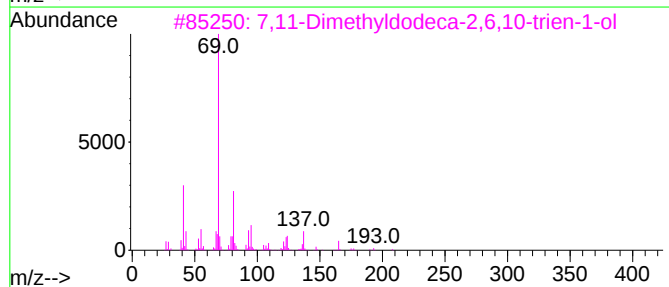
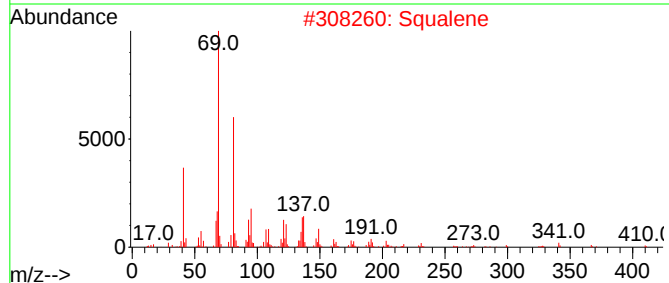
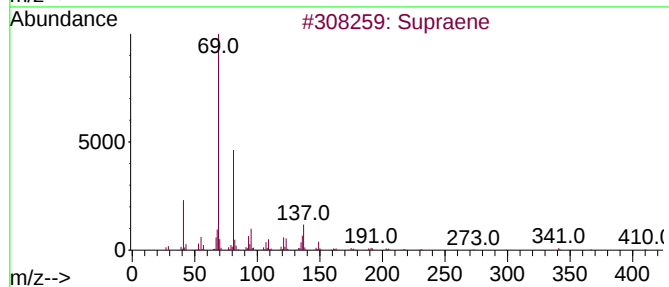
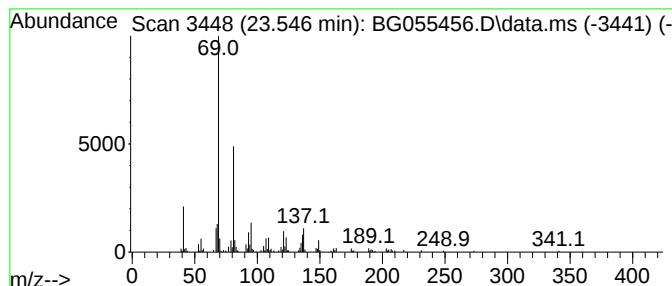
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 5 Supraene Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 23.546 | 7.53 ng | 217226 | Perylene-d12     | 25.227 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|---------|--------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50  | 007683-64-9  | 91   |
| 2    |    |   | Squalene                            | 410 | C30H50  | 000111-02-4  | 90   |
| 3    |    |   | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4  | 87   |
| 4    |    |   | Docosa-2,6,10,14,18-pentaen-22-a... | 384 | C27H44O | 1000163-04-7 | 83   |
| 5    |    |   | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7  | 78   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG110422\  
Data File : BG055456.D  
Acq On : 4 Nov 2022 16:20  
Operator : CG/JU  
Sample : N5306-10  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
DISSOLVED-20221174-COMP-09-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG110122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.274  | 4.7     | ng    | 35517    | 1                     | 8.235  | 150464 | 20.0 |
| Ethanol, 2-(2-b... | 10.808 | 8.2     | ng    | 88759    | 2                     | 11.061 | 216380 | 20.0 |
| n-Hexadecanoic ... | 18.435 | 2.5     | ng    | 57290    | 4                     | 17.583 | 455406 | 20.0 |
| n-Nonadecanol-1    | 21.461 | 4.1     | ng    | 110134   | 5                     | 21.854 | 538645 | 20.0 |
| Supraene           | 23.546 | 7.5     | ng    | 217226   | 6                     | 25.227 | 576626 | 20.0 |